Day 4: Classification

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Introduction to Data Science and Big Data Analytics

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Day 4 Outline

Classification

Maximum Likelihood

Logistic regression with several variables

Confounding

Logistic regression with more than two classes

Discriminant Analysis
- Bayes theorem for classification
- Linear Discriminant Analysis when $p > 1$
- Characterizing performance of classifiers
- Other forms of Discriminant Analysis
- Naive Bayes Classifier

Logistic Regression versus LDA

Classification

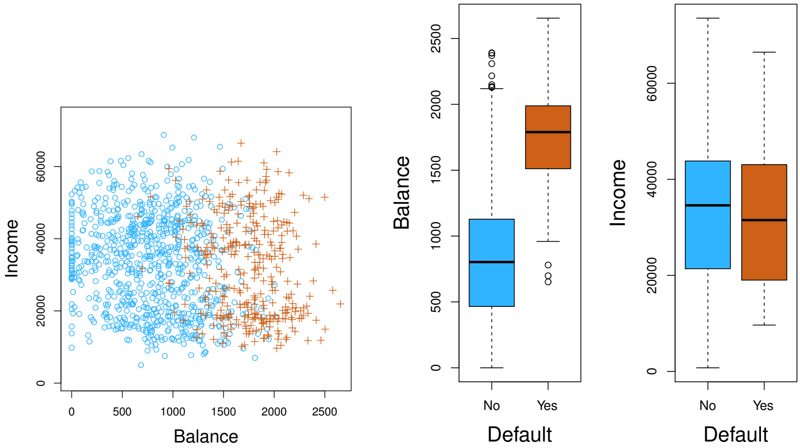
Classification

- Qualitative variables take values in an unordered set $\mathcal{C}$, such as: *eye color* $\in$ {*brown,blue,green*}; *email* $\in$ {*spam, ham*}.
- Given a feature vector X and a qualitative response Y taking values in the set $\mathcal{C}$, the classification task is to build a function $\mathcal{C}(\mathcal{X})$ that takes as input the feature vector X and predicts its value for Y; i.e. $\mathcal{C}(\mathcal{X}) \in \mathcal{C}$.

Classification

- Often we are more interested in estimating the probabilities that X belongs to each category in $\mathcal{C}$.
- For example, it is more valuable to have an estimate of the probability that an insurance claim is fraudulent, than a classification fraudulent or not.

Example: Credit Card Default



Can we use Linear Regression?

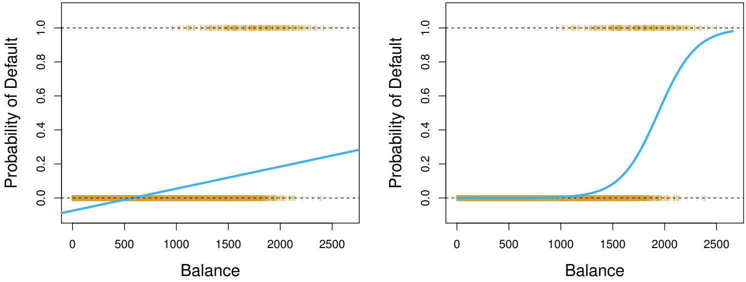
Suppose for the Default classification task that we code

$$Y = \begin{cases} 0 & \text{if } No \\ 1 & \text{if } Yes. \end{cases}$$

Can we simply perform a linear regression of Y on X and classify as Yes if $\hat{Y} > 0.5$?

- In this case of a binary outcome, linear regression does a good job as a classifier, and is equivalent to linear discriminant analysis which we discuss later.
- Since in the population $E(Y|X = x) = Pr(Y = 1|X = x)$, we might think that regression is perfect for this task.
- However, linear regression might produce probabilities less than zero or bigger than one. Logistic regression is more appropriate.

Linear versus Logistic Regression



- The orange marks indicate the response Y, either 0 or 1.
- Linear regression does not estimate $Pr(Y = 1|X)$ well.
- Logistic regression seems well suited to the task.

Linear Regression continued

- Now suppose we have a response variable with three possible values. A patient presents at the emergency room, and we must classify them according to their symptoms.

$$Y = \begin{cases} 1 & \text{if } \textit{stroke}; \\ 2 & \text{if } \textit{drug overdose}; \\ 3 & \text{if } \textit{epileptic seizure}. \end{cases}$$

- This coding suggests an ordering, and in fact implies that the difference between *stroke* and *drug overdose* is the same as between *drug overdose* and *epileptic seizure*.
- Linear regression is not appropriate here.
- Multiclass Logistic Regression or Discriminant Analysis are more appropriate.

Logistic Regression

- Let's write $p(X) = Pr(Y = 1|X)$ for short and consider using *balance* to predict *default*. Logistic regression uses the form

$$p(X) = \frac{e^{\beta_0+\beta_1 X}}{1 + e^{\beta_0+\beta_1 X}}.$$

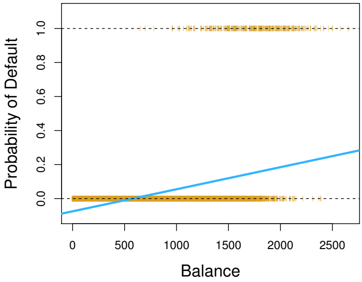
($e \approx 2.71828$ is a mathematical constant [Euler's number.])

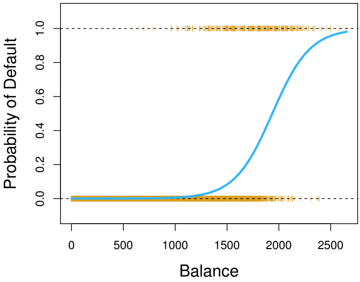
- It is easy to see that no matter what values β_0, β_1 or X take, $p(X)$ will have values between 0 and 1.
- A bit of rearrangement gives

$$log\left(\frac{p(X)}{1 - p(X)}\right) = \beta_0 + \beta_1 X.$$

- This monotone transformation is called the log odds or logit transformation of $p(X)$.

Linear versus Logistic Regression





- Logistic regression ensures that our estimate for $p(X)$ lies between 0 and 1.

Maximum Likelihood

- We use maximum likelihood to estimate the parameters.

$$\ell(\beta_0, \beta) = \prod_{i:y_i=1} p(x_i) \prod_{i:y_i=0} (1 - p(x_i)).$$

- This likelihood gives the probability of the observed zeros and ones in the data.
- We pick β_0 and β_1 to maximize the likelihood of the observed data.
- Most statistical packages can fit linear logistic regression models by maximum likelihood. In R we use the *glm* function.

```r
library(ISLR)
data("Default")
names(Default)

## [1] "default" "student" "balance" "income"

logit <- glm(Default$default ~ Default$balance, family = binomial)
```

```r
summary(logit)
```

```
##
## Call:
## glm(formula = Default$default ~ Default$balance, family = binomial)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -2.2697  -0.1465  -0.0589  -0.0221   3.7589
##
## Coefficients:
##                   Estimate Std. Error z value Pr(>|z|)
## (Intercept)     -1.065e+01  3.612e-01  -29.49   <2e-16 ***
## Default$balance  5.499e-03  2.204e-04   24.95   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2920.6  on 9999  degrees of freedom
## Residual deviance: 1596.5  on 9998  degrees of freedom
## AIC: 1600.5
##
## Number of Fisher Scoring iterations: 8
```

Making Predictions

- What is our estimated probability of *default* for someone with a balance of \$1000?

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 X}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 X}} = \frac{e^{-10.6513 + 0.0055 \times 1000}}{1 + e^{-10.6513 + 0.0055 \times 1000}} = 0.006$$

- With a balance of \$2000?

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 X}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 X}} = \frac{e^{-10.6513 + 0.0055 \times 2000}}{1 + e^{-10.6513 + 0.0055 \times 2000}} = 0.586$$

```r
logit2 <- glm(Default$default ~ Default$student, family = binomial)
summary(logit2)
```

```
##
## Call:
## glm(formula = Default$default ~ Default$student, family = binomial)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -0.2970  -0.2970  -0.2434  -0.2434   2.6585
##
## Coefficients:
##                     Estimate Std. Error z value Pr(>|z|)
## (Intercept)         -3.50413    0.07071  -49.55  < 2e-16 ***
## Default$studentYes   0.40489    0.11502    3.52 0.000431 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2920.6  on 9999  degrees of freedom
## Residual deviance: 2908.7  on 9998  degrees of freedom
## AIC: 2912.7
##
## Number of Fisher Scoring iterations: 6
```

Making Predictions (binary variable)

$$\widehat{Pr}(default = Yes|student = Yes) = \frac{e^{-3.5041+0.4049\times 1}}{1+e^{-3.5041+0.4049\times 1}} = 0.0431$$

$$\widehat{Pr}(default = Yes|student = No) = \frac{e^{-3.5041+0.4049\times 0}}{1+e^{-3.5041+0.4049\times 0}} = 0.0292$$

Logistic regression with several variables

$$log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p$$

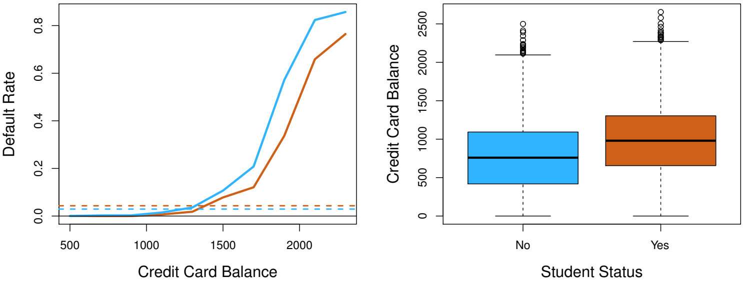
$$p(X) = \frac{e^{\beta_0+\beta_1 X_1+\ldots+\beta_p X_p}}{1+e^{\beta_0+\beta_1 X_1+\ldots+\beta_p X_p}}$$

```r
logit3 <- glm(Default$default ~ Default$balance + Default$income + Default$stud
summary(logit3)
```

```
##
## Call:
## glm(formula = Default$default ~ Default$balance + Default$income +
##     Default$student, family = binomial)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -2.4691  -0.1418  -0.0557  -0.0203   3.7383
##
## Coefficients:
##                      Estimate Std. Error z value Pr(>|z|)
## (Intercept)        -1.087e+01  4.923e-01 -22.080  < 2e-16 ***
## Default$balance     5.737e-03  2.319e-04  24.738  < 2e-16 ***
## Default$income      3.033e-06  8.203e-06   0.370  0.71152
## Default$studentYes -6.468e-01  2.363e-01  -2.738  0.00619 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2920.6  on 9999  degrees of freedom
## Residual deviance: 1571.5  on 9996  degrees of freedom
## AIC: 1579.5
##
## Number of Fisher Scoring iterations: 8
```

- Why is coefficient for *student* negative, while it was positive before?

Confounding



- Students tend to have higher balances than non-students, so their marginal default rate is higher than for non-students.
- But for each level of balance, students default less than non-students.
- Multiple logistic regression can tease this out.

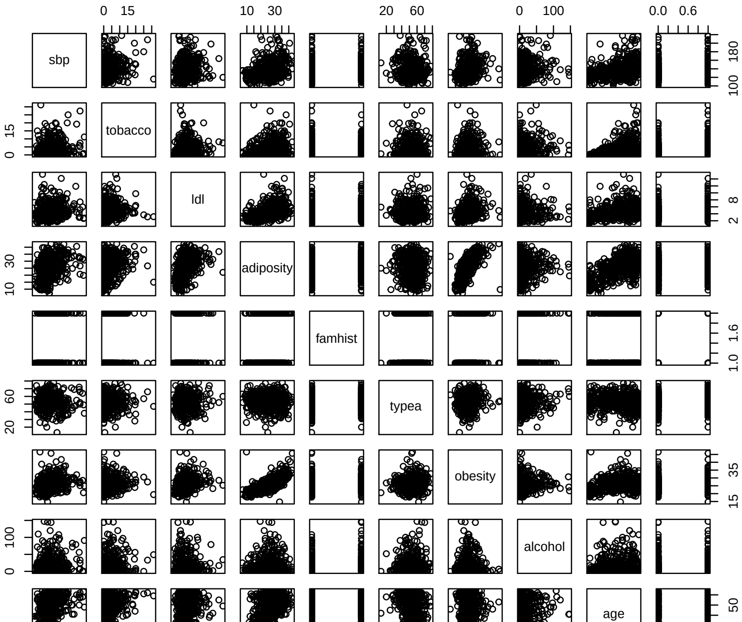
Example: South African Heart Disease

- 160 cases of MI (myocardial infarction) and 302 controls (all male in age range 15-64), from Western Cape, South Africa in early 80s.
- Overall prevalence very high in this region: 5.1%.
- Measurements on seven predictors (risk factors), shown in scatterplot matrix.
- Goal is to identify relative strengths and directions of risk factors.
- This was part of an intervention study aimed at educating the public on healthier diets.

```r
library(ElemStatLearn)
data("SAheart")
names(SAheart)

##  [1] "sbp"       "tobacco"   "ldl"       "adiposity" "famhist"
##  [6] "typea"     "obesity"   "alcohol"   "age"       "chd"
```

```r
pairs(SAheart)
```



```
heartfit <- glm(chd ~ . , data = SAheart, family = binomial)
summary(heartfit)

##
## Call:
## glm(formula = chd ~ ., family = binomial, data = SAheart)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.7781  -0.8213  -0.4387   0.8889   2.5435
##
## Coefficients:
##                 Estimate Std. Error z value Pr(>|z|)
## (Intercept)    -6.1507209  1.3082600  -4.701 2.58e-06 ***
## sbp             0.0065040  0.0057304   1.135 0.256374
## tobacco         0.0793764  0.0266028   2.984 0.002847 **
## ldl             0.1739239  0.0596617   2.915 0.003555 **
## adiposity       0.0185866  0.0292894   0.635 0.525700
## famhistPresent  0.9253704  0.2278940   4.061 4.90e-05 ***
## typea           0.0395950  0.0123202   3.214 0.001310 **
## obesity        -0.0629099  0.0442477  -1.422 0.155095
## alcohol         0.0001217  0.0044832   0.027 0.978350
## age             0.0452253  0.0121298   3.728 0.000193 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
```

Logistic regression with more than two classes

- So far we have discussed logistic regression with two classes.
- It is easily generalized to more than two classes.
- One version (used in the R package *glmnet*) has the symmetric form

$$Pr(Y = k|X) = \frac{e^{\beta_{0k}+\beta_{1k}X_1+\ldots+\beta_{pk}X_p}}{\sum_{\ell=1}^{K} e^{\beta_{0\ell}+\beta_{1\ell}X_1+\ldots+\beta_{p\ell}X_p}}$$

- Here there is a linear function for each class.
- Multiclass logistic regression is also referred to as multinomial regression.

Discriminant Analysis

- Here the approach is to model the distribution of X in each of the classes separately, and then use Bayes theorem to flip things around and obtain $Pr(Y|X)$.
- When we use normal (Gaussian) distributions for each class, this leads to linear or quadratic discriminant analysis.
- However, this approach is quite general, and other distributions can be used as well. Here, we will focus on normal distributions.

Bayes theorem for classification

- Thomas Bayes was a famous mathematician whose name represents a big subfield of statistical and probabilistic modeling.
- Here we focus on a simple result, known as Bayes theorem:

$$Pr(Y = k|X = x) = \frac{Pr(X = x|Y = k) \cdot Pr(Y = k)}{Pr(X = x)}$$

- One writes this slightly differently for discriminant analysis:

$$Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)},$$

  where
  - $f_k(x) = Pr(X = x|Y = k)$ is the density for X in class k. Here we will use normal densities for these, separately in each class.
  - $\pi_k = Pr(Y = k)$ is the marginal or prior probability for class k.

Why discriminant analysis?

- When the classes are well-separated, the parameter estimates for the logistic regression model are surprisingly unstable. Linear discriminant analysis does not suffer from this problem.
- If n is small and the distribution of the predictors X is approximately normal in each of the classes, the linear discriminant model is again more stable than the logistic regression model.
- Linear discriminant analysis is popular when we have more than two response classes, because it also provides low-dimensional views of the data.

Linear Discriminant Analysis when $p = 1$

- The Gaussian density has the form

$$f_k(x) = \frac{1}{\sqrt{2\pi\sigma_k}} e^{-\frac{1}{2}\left(\frac{x-\mu_k}{\sigma_k}\right)^2}$$

- Here μ_k is the mean, and σ_k^2 the variance (in class k). We will assume that all the $\sigma_k = \sigma$ are the same.
- Plugging this into Bayes formula, we get a rather complex expression for $p_k(x) = Pr(Y = k|X = x)$:

$$f_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{1}{2}\left(\frac{x-\mu_k}{\sigma}\right)^2}}{\sum_{\ell=1}^{K} \pi_\ell \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{1}{2}\left(\frac{x-\mu_\ell}{\sigma}\right)^2}}$$

- There are simplifications and cancellations.

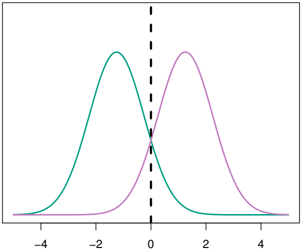
Discriminant functions

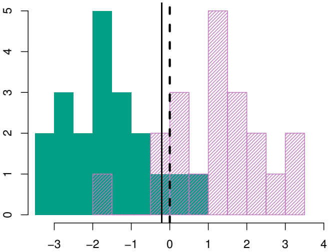
- To classify at the value $X = x$, we need to see which of the $p_k(x)$ is largest. Taking logs, and discarding terms that do not depend on k, we see that this is equivalent to assigning x to the class with the largest discriminant score:

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + log(\pi_k)$$

- Note that $\delta_k(x)$ is a linear function of x.
- If there are $K = 2$ classes and $\pi_1 = \pi_2 = 0.5$, then one can see that the decision boundary is at

$$x = \frac{\mu_1 + \mu_2}{2}.$$



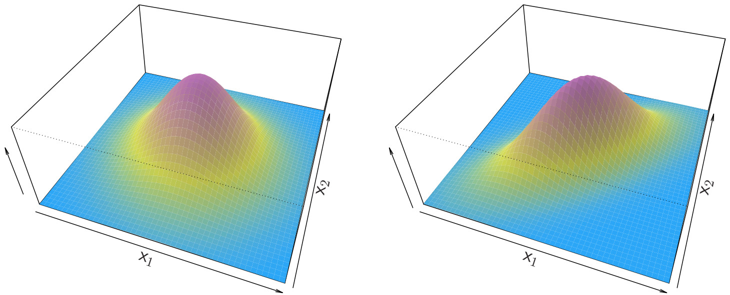


- Example with $\mu_1 = -1.5,\ \mu_2 = 1.5,\ \pi_1 = \pi_2 = 0.5$,and $\sigma^2 = 1$.
- Typically we don't know these parameters; we just have the training data.
- In that case we simply estimate the parameters and plug them into the rule.

Estimating the parameters

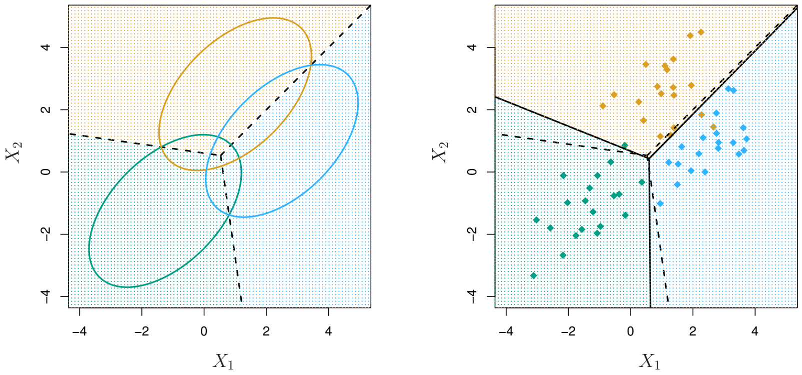
- $\hat{\pi}_k = \frac{n_k}{n}$;
- $\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i$;
- $\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2 = \sum_{k=1}^{K} \frac{n_k-1}{n-K} \cdot \hat{\sigma}_k^2$
- where $\hat{\sigma}_k^2 = \frac{1}{n_k-1} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2$ is the usual formula for the estimated variance in the kth class.

Linear Discriminant Analysis when $p > 1$



- Density: $f(x) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} e^{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)}$
- Discriminant function:
  $\delta_k(x) = x^T\Sigma^{-1}\mu_k - \frac{1}{2}\mu_k^T\Sigma^{-1}\mu_k + log\pi_k$
- Despite its complex form,
  $\delta_k(x) = c_{k0} + c_{k1}x_1 + c_{k2}x_2 + \cdots + c_{kp}x_p$ – a linear function.

Illustration: $p = 2$ and $K = 3$ classes



- Here $\pi_1 = \pi_2 = \pi_3 = 1/3$.
- The dashed lines are known as the Bayes decision boundaries.
- Were they known, they would yield the fewest misclassification errors, among all possible classifiers.

From $\delta_k(x)$ to probabilities

- Once we have estimates $\delta_k(x)$, we can turn these into estimates for class probabilities:

$$\widehat{Pr}(Y = k|X = x) = \frac{e^{\hat{\delta}_k(x)}}{\sum_{\ell=1}^{K} e^{\hat{\delta}_\ell(x)}}.$$

- So classifying to the largest $\hat{\delta}_k(x)$ amounts to classifying to the class for which $\widehat{Pr}(Y = k|X = x)$ is largest.
- When $K = 2$, we classify to class 2 if $\widehat{Pr}(Y = 2|X = x) \geq 0.5$, else to class 1.

Confusion matrix and error rates

		True No	Default Yes	Status Total
Predicted	No	9644	252	9896
Default Status	Yes	23	81	104
	Total	9667	333	10000

- (23 + 252) / 10000 errors — a 2.75% misclassification rate.
- Some caveats:
  - This is training error, and we may be overfitting. Not a big concern here since $n = 10000$ and $p = 4$.
  - If we classified to the prior – always to class *No* in this case – we would make 333/10000 errors, or only 3.33%.
  - Of the true *No*'s, we make $23/9667 = 0.2\%$ errors; of the true *Yes*'s, we make $252/333 = 75.7\%$ errors!

Types of errors

- False positive rate: The fraction of negative examples that are classified as positive – 0.2% in example.
- False negative rate: The fraction of positive examples that are classified as negative – 75.7% in example.

Sensitivity and specificity

- Performance of a classifier is often characterized in terms of sensitivity and specificity.
- Here, the sensitivity is the percentage of true defaulters that are identified. It is 24.3% in our case.
- The specificity is the percentage of non-defaulters that are correctly identified. Here it is $(1 - 23/9,667) \cdot 100 = 99.8\%$
- The true positive rate is the sensitivity of our classifier.
- The false positive rate is *one minus* the specificity of our classifier.

Errors and threshold

- We produced the confusion matrix above by classifying to class *Yes* if

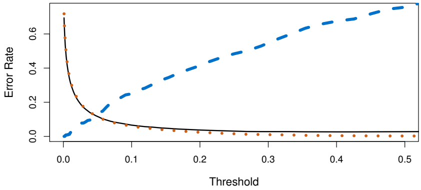
$$\widehat{Pr}(Default = Yes|Balance, Student) \geq 0.5$$

- We can change the two error rates by changing the threshold from 0.5 to some other value in [0,1]:

$$\widehat{Pr}(Default = Yes|Balance, Student) \geq threshold,$$

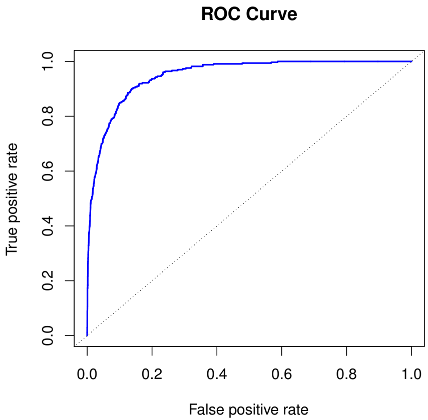
and vary *threshold*.

Varying the *threshold*



- Error rates are shown as a function of the threshold value for the posterior probability that is used to perform the assignment.
- The black solid line displays the overall error rate.
- The blue dashed line represents the fraction of defaulting customers that are incorrectly classified (False Negative).
- The orange dotted line indicates the fraction of errors among the non-defaulting customers (False Positive).
- In order to reduce the false negative rate, we may want to reduce the threshold to 0.1 or less.

ROC curve



- The ROC plot displays both simultaneously.
- Sometimes we use the AUC or area under the curve to summarize the overall performance.
- Higher AUC is good.

Characterizing performance of classifiers

		Predicted	class	
		- or Null	+ or Non-null	Total
True	- or Null	True Neg. (TN)	False Pos.(FP)	N
class	+ or Non-null	False Neg. (FN)	True Pos. (TP)	P
	Total	N*	P*	

- "+" is "disease" or alternative (non-null) hypothesis (here, those who default);
- "-" is "non-disease" or the null hypothesis (here, those who do not default).

Performance measures for classifiers

Name	Definition	Synonyms
False Pos. rate	FP/N	Type I error, 1- Specificity
True Pos. rate	TP/P	1 - Type II error, power, sensitivity, recall
Pos. Pred. value	TP/P*	Precision, 1-false discovery proportion
Neg. Pred. value	TN/N*	

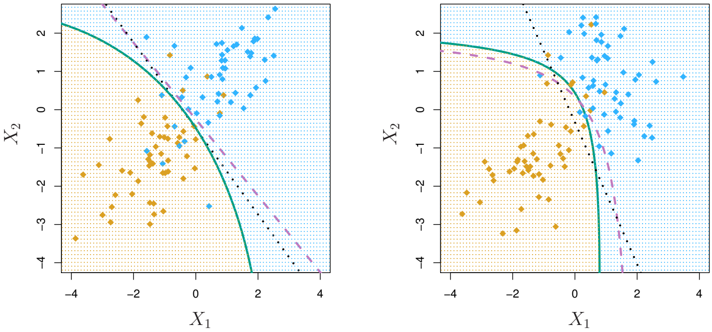
- The denominators for the false positive and true positive rates are the actual population counts in each class.
- The denominators for the positive predictive value and the negative predictive value are the total predicted counts for each class.

Other forms of Discriminant Analysis

$$Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{\ell=1}^{K} \pi_\ell f_\ell(x)}$$

- When $f_k(x)$ are Gaussian densities, with the same covariance matrix Σ in each class, this leads to linear discriminant analysis.
- By altering the forms for $f_k(x)$, we get different classifiers.
  - With Gaussians but different Σ_k in each class, we get quadratic discriminant analysis.
  - With $f_k(x) = \prod_{j=1}^{p} f_{jk}(x_j)$ (conditional independence model) in each class we get naive Bayes. For Gaussian this means the Σ_k are diagonal.
  - Many other forms, by proposing specific density models for $f_k(x)$, including nonparametric approaches.

Quadratic Discriminant Analysis



- $\delta_k(x) = -\frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k) + log \pi_k$
- Because the Σ_k are different, the quadratic terms matter.

Naive Bayes

- Assumes features are independent in each class.
- Useful when p is large, and so multivariate methods like QDA and even LDA break down.
- Gaussian naive Bayes assumes each Σ_k is diagonal:

$$\delta_k(x) \propto log\left[\pi_k \prod_{j=1}^{p} f_{kj}(x_j)\right] = -\frac{1}{2}\sum_{j=1}^{p}\frac{(x_j-\mu_{kj})^2}{\sigma_{kj}^2} + log\pi_k$$

- Can use for mixed feature vectors (qualitative and quantitative). If X_j is qualitative, replace $f_{kj}(x_j)$ with probability mass function (histogram) over discrete categories.
- Despite strong assumptions, naive Bayes often produces good classification results.

Naive Bayes Classifier

- Naive Bayes (NB) classifier especially appropriate when the dimension p of the feature space is high, making density estimation unattractive.
- Assumes that given a class $G = j$, the features X_k are independent:

$$f_j(X) = \prod_{k=1}^{p} f_{jk}(X_k).$$

- While this assumption is pretty heroic and generally not true, it significantly simplifies the estimation.
- The individual class-conditional marginal densities f_{jk} can each be estimated separately.
- If a component X_j of X is discrete, then an appropriate histogram estimate can be used. This provides a seamless way of mixing variable types in a feature vector.

Naive Bayes Classifier

- Despite these strong assumptions, NB classifiers often outperform far more sophisticated alternatives.
- Although the individual class density estimates may be biased, this bias might not hurt the posterior probabilities as much, especially near the decision regions.
- In fact, the problem may be able to withstand considerable bias for the savings in variance such a “naive” assumption earns.

Logistic Regression versus LDA

- For a two-class problem, one can show that for LDA

$$log\left(\frac{p_1(x)}{1-p_1(x)}\right) = log\left(\frac{p_1(x)}{p_2(x)}\right) = c_0 + c_1x_1 + \cdots + c_px_p$$

- So it has the same form as logistic regression.
- The difference is in how the parameters are estimated.
  - Logistic regression uses the conditional likelihood based on $Pr(Y|X)$ (known as discriminative learning).
  - LDA uses the full likelihood based on $Pr(X, Y)$ (known as generative learning).
  - Despite these differences, in practice the results are often very similar.
- Note: logistic regression can also fit quadratic boundaries like QDA, by explicitly including quadratic terms in the model.

Summary

- Logistic regression is very popular for classification, especially when $K = 2$.
- LDA is useful when n is small, or the classes are well separated, and Gaussian assumptions are reasonable. Also when $K > 2$.
- Naive Bayes is useful when p is very large.
- See Section 4.5 for some comparisons of logistic regression, LDA and KNN.